

Monte Carlo Search for Very Hard KSAT Realizations for Use in Quantum Annealing

T. Neuhaus^a

^a*Jülich Supercomputing Centre, Forschungszentrum Jülich, D-52425 Jülich, Germany*

Abstract

Using powerful Multicanonical Ensemble Monte Carlo methods from statistical physics we explore the realization space of random K satisfiability (KSAT) in search for computational hard problems, most likely the 'hardest problems'. We search for realizations with unique satisfying assignments (USA) at ratio of clause to spin number $\alpha = M/N$ that is minimal. USA realizations are found for α -values that approach $\alpha = 1$ from above with increasing number of spins N . We consider small spin numbers in $2 \leq N \leq 18$. The ensemble mean exhibits very special properties. We find that the density of states of the first excited state with energy one $\Omega_1 = g(E = 1)$ is consistent with an exponential divergence in N : $\Omega_1 \propto \exp[+rN]$. The rate constants for $K = 2, 3, 4, 5$ and $K = 6$ of KSAT with USA realizations at $\alpha = 1$ are determined numerically to be in the interval $r = 0.348$ at $K = 2$ and $r = 0.680$ at $K = 6$. These approach the unstructured search value $\ln 2$ with increasing K . Our ensemble of hard problems is expected to provide a test bed for studies of quantum searches with Hamiltonians that have the form of general Ising models.

Keywords: Spin Glass, Monte Carlo, Quantum Adiabatic Computation

1. Introduction

Random satisfiability problems like three satisfiability (3SAT) and its generalization KSAT form a corner stone of complexity theory, a very active research branch in formal logic and computer science. In these theories one is concerned with logical forms $\mathcal{F}(X)$ defined on some bit space \mathbf{X} and one discusses the question whether or not there exists an assignment \mathbf{X}_0 that turns the value of the logical form $\mathcal{F}(\mathbf{X}_0)$ into "true". The decision problem of KSAT and its accompanying function problem: the actual calculation of \mathbf{X}_0 at given $\mathcal{F}(\mathbf{X})$ for $K \geq 3$ belong to the class of NP complete theories [1], which for all practical purposes implies computational intractability. In these theories it is very common that worst case realization ensembles of forms $\mathcal{F}(\mathbf{X})$ exhibit an algorithm dependent complexity C , that rises exponentially $C \propto \exp[+rN]$ with the number of bits N . The rate constants r are smaller than the unstructured search value $r = \ln 2$ but at the same time can take values that are finite fractions of $\ln 2$. This implies, that there exist problems which are not solvable even for small

numbers of bits like $N = 100$, neither by analytic nor numeric methods, even using brute computational force.

It is the privilege of statistical physics to turn the abstract notion of satisfiability into studies of Hamiltonian systems upon mapping the bit degrees of freedom $X_i = 0, 1$ via $s_i = 2X_i - 1$ for $i = 1, \dots, N$ to Ising degrees of freedom $s_i \pm 1$, and upon introducing a suitable Hamiltonian H_{KSAT} whose ground-states at energy $E = 0$ map one by one to the satisfying assignments of $\mathcal{F}(\mathbf{X})$. One may either consider classical statistical physics where the theory is supplied by artificial thermal fluctuations at inverse temperature $\beta = T^{-1}$ within the framework of the canonical partition function $Z_C = \sum_{\text{Conf.}} \exp[-\beta H_{\text{KSAT}}]$ or alternatively, consider the quantum statistical theory of Pauli spins S_i^x, S_i^y and S_i^z with the quantum partition function

$$Z_Q = \text{Tr} \langle \Psi | \exp[-\beta[(1 - \lambda) \sum_i S_i^x + \lambda H_{\text{KSAT}}(S_i^z)]] | \Psi \rangle, \quad (1.1)$$

where quantum fluctuations at low $T \approx 0$ are tuned via an external parameter λ . For both cases the mathematical intractability is encoded into physical theories and it is an exciting research topic to study its consequences i.e., phase transitions and correlations from various points of view. For the classical theory it was shown, that computational intractability is related to a phase transition - the SAT transition - along the principal parameter direction $\alpha = M/N$ of random KSAT theories [2], the ratio α hereby denoting the ratio of clause M to spin N numbers. In a later effort complexity related observables were determined analytically within the framework of replica symmetry breaking theory for random 3SAT [3], and also numerically in large scale simulations [4]. In particular the critical point of the 3SAT transition was determined to be $\alpha_S = 4.267\dots$ analytically. For the quantum theory, and within quantum information theory it was conjectured that adiabatic quantum computations (AQC) based on the properties of Z_Q could possibly obtain ground states of H_{KSAT} in polynomial physical time [5, 6]. For hard 3SAT realizations it turned out however, that early findings on polynomial ground state search times had to be corrected to exponentially large ones [7] for the simplest case of AQC making use of a transverse magnetic field and a linear λ -parameter schedule. A similar finding was made recently for a another satisfiability theory: Exact Cover [8].

Within the current work we execute a very use-full exercise prior to the actual studies of complexity related observables in physical theories. We restrict the admissible set of all KSAT Hamiltonians, namely random KSAT realizations with ensemble mean $\langle \dots \rangle_{\text{RANDOM KSAT}}$, to a much smaller 'hard' set $\langle \dots \rangle_{\text{HARD}}$ of H_{KSAT}^η Hamiltonian's with corresponding ensemble mean. The index η denotes the ensemble members which for reasons of computer time limitations have finite number $\eta = 1, \dots, 1000$ throughout the paper. As far as ground-state searches are concerned our problem set is targeted at hard problems - most likely the 'hardest problems' - which otherwise and within $\langle \dots \rangle_{\text{RANDOM KSAT}}$ are exponentially rare. Our problems are constructed under specific constraints:

- The ground-state to any H_{KSAT}^η is unique, which if $g^\eta(E)$ denotes the density of states

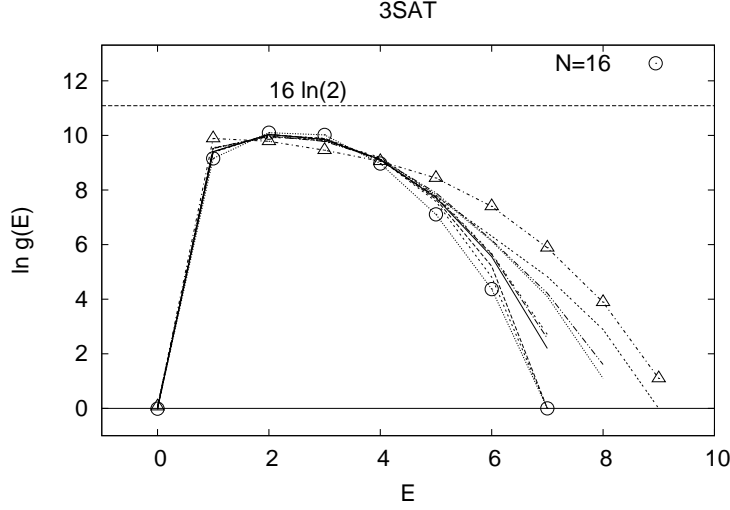


Figure 1: We display an example for Logarithmic scale density of states functions $g^\eta(E)$ for $\eta = 1, \dots, 10$ realizations for the theory 3SAT at $N = 16$ spins. Density of states functions have finite support integer values but for optical reconnaissance reasons are connected with polygons. Some functional values are identified by circles and triangles. It is remarkable: the density of states jumps from $g(E = 0) = 1$ (USA) to a large value $\Omega_1 = g(E = 1) \approx e^{9.3} \approx 11000$. As far as ground-state searches are concerned: any stochastic ground-state search can easily reach the $E = 1$ surface. Beyond that and in front of $E = 0$ the search has to enumerate an exponential large number of possibilities.

function (DOS) implies $g^\eta(E = 0) = 1$. Such problem realizations possess unique satisfying assignment's (USA).

- For a given number of spins N and for realizations with $g(E = 0) = 1$ the number of clauses M is minimal. The parameter α is then minimal too $\alpha = \alpha_{min}$. E.g. : we find that USA realizations in 3SAT for α_{min} follow $\alpha_{min} = (N + 4)/N$.
- The set of problem realizations $\langle \dots \rangle_{\text{HARD}}$ is drawn with unique probability from the set of $\langle \dots \rangle_{\text{RANDOM KSAT}}$ realizations.

Similar realizations have lately been considered for 3SAT in Ref. [9] with a weaker constraint on the value α , which had the value $\alpha = 3$. The minimal KSAT values within this work turn out to approach $\alpha_{min} = 1$ from above independent of K with increasing N . In short: we are constructing USA realizations in KSAT at $\alpha = 1$ asymptotically.

At the heart of our numerical calculations is a Markov Chain Monte Carlo study of the partition function

$$\Gamma(\mu) = \mathcal{N}^{-1} \sum_{\text{Random KSAT}} \delta^{(1)}[\mu - g(E = 0)], \quad (1.2)$$

which partitions the realization space of random KSAT within respect to μ , the ground-state multiplicity. Once the Markov Chain Monte Carlo visits the $\mu = 1$ sector (USA) corresponding problems are collected on the disk of a computer. Similar flat histogram sampling

methods, like Wang-Landau [10] and Multicanonical [11] simulations have recently been used in complexity theory in an attempt to sample the density of states function $g(E)$ in 3SAT for spin numbers N that prohibit exact enumeration [12]. The final part of the paper classifies measures of complexity within typical problem realizations in $\langle \dots \rangle_{\text{HARD}}$.

Today's understanding on the origin on the complexity of the physical search in frustrated and disordered systems pictures a free energy landscape in which as a function of the value N , a finite number of solution clusters is accompanied by an exponentially large number of almost solution clusters at energy near but above the ground-state. All clusters are separated by finite free energy barriers. The situation resembles the search for a needle - or several needles - in a haystack. A simplified mechanism operates within our hard problem ensemble $\langle \dots \rangle_{\text{HARD}}$. We find, that the phase space volume Ω_1 at $E = 1$ is exponentially large in the number of degrees of freedom N , see the examples of $g(E)$ displayed in Fig.(1). Thus first: for all of the considered KSAT theories with $K = 2$ up to $K = 6$ we encounter the generic situation: a single needle is searched in a haystack of exponential large size¹. Second: we find numeric evidence that actual values of Ω_1 are extremal i.e., maximal under the condition of minimal α , which in turn justifies the notion of most likely the 'hardest problems'.

2. Theory, Hard Problems and Monte Carlo Simulation

2.1. Theory and Observables

In KSAT one considers logical forms \mathcal{F} - a function - whose truth value can either be true or false and which are defined on a space of N Boolean degrees of freedom - bits - X_i with $i = 1, \dots, N$. In the satisfiability problem one asks for the existences of assignment's i.e., bits \mathbf{X}_0 that would evaluate the function \mathcal{F} at the value true. Solving the function problem implies the explicit calculation of a single satisfying assignment or, of all different satisfying assignments if there are several of those. The logical form \mathcal{F} is the conjunctive normal form of M clauses $\{C_1, \dots, C_M\}$: $\mathcal{F} = C_1 \wedge C_2 \wedge \dots \wedge C_M$, which only evaluates true if all clauses C_α with $\alpha = 1, \dots, M$ evaluate true simultaneously. Any of the M clauses is the disjunction of integer K literals $L_{\alpha,j}$ with $K \geq 2$ and $j = 1, \dots, K$:

$$C_\alpha = L_{\alpha,1} \vee L_{\alpha,2} \vee \dots \vee L_{\alpha,K}. \quad (2.1)$$

A clause is true, if at least one of its literals evaluates true. For example, in 3SAT there are 7 configurations of literals on the clause which evaluate true and just one with truth value false. In addition, a literal is either a bit X or its negation \overline{X} and, the actual identification of a literal with a specific bit - or its negation - is controlled by a map $(\alpha, j) \rightarrow i : i = i[\alpha, j]$, that associates clauses and clause-positions α, j to the index set i of bits. The map $i = i[\alpha, j]$ and the possibility of 2^{KM} negations at the literal positions are free parameters of the theory.

¹The theories at $K \geq 3$ are NP-complete while at $K = 2$ there exist mathematical polynomial time algorithms that find the ground-state even though Ω_1 is exponentially large.

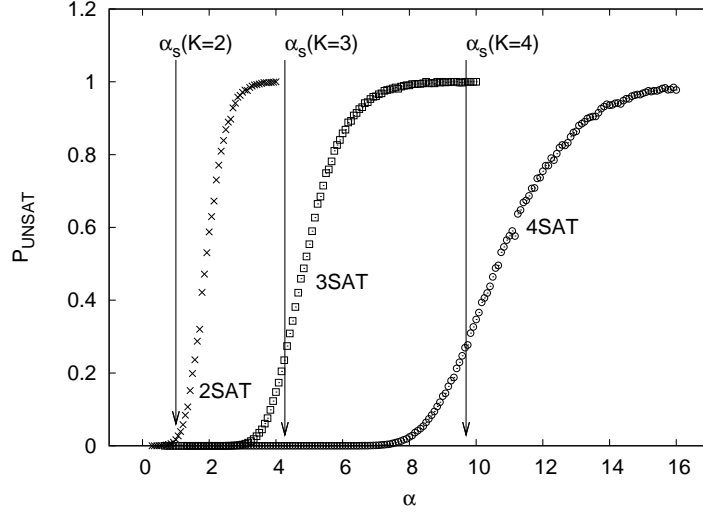


Figure 2: Probability P_{UNSAT} of un-satisfiable formulas within $\langle \dots \rangle_{\text{RANDOM KSAT}}$ for $K = 2, 3$ and $K = 4$ als a function of α . Exact and numerical values for the SAT to UNSAT threshold $\alpha_s(K)$ are indicated by arrows. The numerical data are obtained from the partition function $\Gamma(\mu)$ of eq.(2.15) via eq.(2.18).

In an Hamiltonian theory they can be used to introduce ensembles with mean $\langle \dots \rangle$ over random disorder as well as random frustration, a possibility that is heavily exploited in this work. It is implicitly understood, that tautologies i.e., contradicting pairs within clauses like $X_i \bar{X}_i$ as well as redundancies i.e., duplicate literals like $X_i X_i$ or $\bar{X}_i \bar{X}_i$ are not admitted to the theory.

The physical degrees of freedom are classical Ising spins $s_i = \pm 1$ with $i = 1, \dots, N$ and without loss of generality, true on each bit X_i is identified with spin up $s_i = +1$. Let us introduce functions h_α in an attempt to write the Hamiltonian H_{KSAT} as a sum of M terms: $H_{\text{KSAT}} = \sum_\alpha h_\alpha$, where each term corresponds to a clause and, where the ground-states of H_{KSAT} at energy $E = 0$ can be identified one by one with the satisfying assignments of \mathcal{F} . For this purpose we note that K spins s_1, \dots, s_K of the clause $C = X_1 \vee X_2 \vee \dots \vee X_K$ add up to the sum $\Sigma = \sum_{i=1}^K s_i$, which takes $K+1$ different values $\Sigma = -K, -K+2, \dots, K-2, K$. Consequently the polynomial $h = h(s_1, \dots, s_K)$

$$h = \frac{(-1)^K}{2^K K!} \prod_{m=1}^K \left(\sum_{i=1}^N s_i + K - 2m \right) \quad (2.2)$$

has the value $h = 0$ for all spin configurations except one, if only all spins are down: $s_i = -1$ with $i = 1, \dots, N$. For the latter case $h = 1$, which implies an energy-gap of value unity. For $K \geq 2$ the function h is a linear combination of the spins n -point functions $\Gamma^0, \Gamma^1, \dots, \Gamma^K$ with a maximum n of value $n_{\text{max}} = K$. For purposes of illustration we present the 2SAT and 3SAT cases. For 2SAT we obtain the anti-ferromagnet at finite field

$$h_{2\text{SAT}} = \frac{1}{4} [s_1 s_2 - (s_1 + s_2) + 1], \quad (2.3)$$

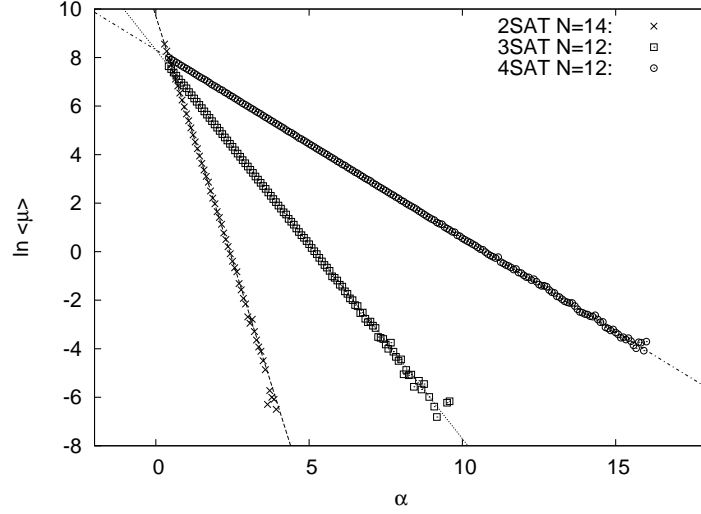


Figure 3: Monte Carlo data for $\ln \langle \mu \rangle$ of random KSAT in accord with eq.(2.16) for selected N values as a function of α and for $K = 2, 3$ and $K = 4$. The straight lines match the Monte Carlo data and correspond to the exact result of eq.(2.17).

while in 3SAT

$$h_{3\text{SAT}} = \frac{1}{8} [s_1 s_2 s_3 + (s_1 s_2 + s_1 s_3 + s_2 s_3) + (s_1 + s_2 + s_3) - 1]. \quad (2.4)$$

The necessary frustrations are encoded in a matrix array $\epsilon_{\alpha,j} = \pm 1$ which for each clause α and position j with $j = 1, \dots, K$ follows the pattern of negations within \mathcal{F} , a negation induces an $\epsilon = -1$ while otherwise $\epsilon = +1$. We mention that in random KSAT, which we denote by the ensemble mean $\langle \dots \rangle_{\text{RANDOM KSAT}}$, values of ϵ are drawn with equal probability $p(\epsilon = +1) = p(\epsilon = -1) = \frac{1}{2}$. The final form of the KSAT Ising Hamiltonian H_{KSAT} is

$$H_{\text{KSAT}} = \sum_{\alpha=1}^M h_{\text{KSAT}}(\epsilon_{\alpha,1} s_{i[\alpha,1]}, \epsilon_{\alpha,2} s_{i[\alpha,2]}, \dots, \epsilon_{\alpha,K-1} s_{i[\alpha,K-1]}, \epsilon_{\alpha,K} s_{i[\alpha,K]}), \quad (2.5)$$

and is the basis of our studies. Its principal parameters for K are the ratio of clause numbers M over N namely $\alpha = M/N$, and the particular assignments of spins to clauses via the map $i[\alpha, j]$, as well as the settings within the frustration matrix $\epsilon_{\alpha,j} = \pm 1$. We denote a specific setting of the latter map and matrix a realization and study ensemble mean expectation values of observables at fixed α throughout the paper.

Once the Hamiltonian is given we formally define the canonical partition function $Z(\beta) = \sum_{\text{Conf.}} e^{-\beta H}$ which at temperature $T = \beta^{-1}$ allows the definition of physical observables as there are the internal energy $U = \partial_{\beta} \ln Z$, or the specific heat $C_V = \beta^2 \partial_{\beta} U$. The canonical partition function has the spectral representation

$$Z(\beta) = \sum_E g(E) e^{-\beta E}, \quad (2.6)$$

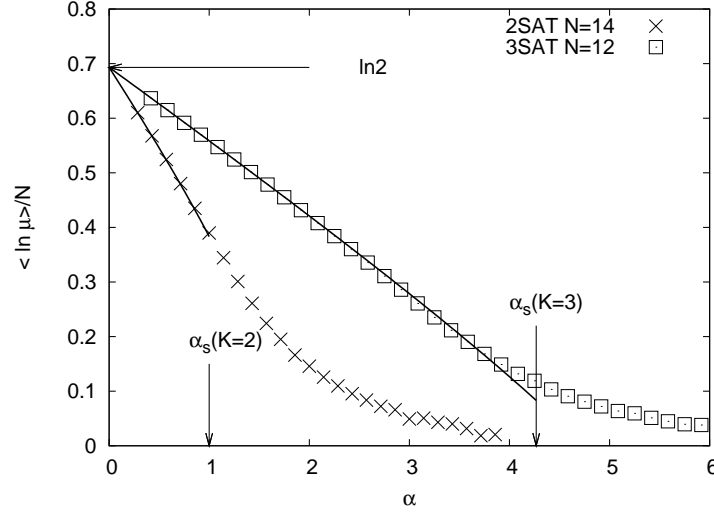


Figure 4: Ground state entropy density $s_0 = \frac{1}{N} \langle \ln \mu \rangle_{\mu>0}$ for random KSAT at $K = 2$ and $K = 3$ as a function of α . The arrows denote exact positions of the SAT to UNSAT threshold at α_s . The data sets are superimposed by series expansion results for s_0 for α -values below α_s . The curves lie on top of the data.

where $g(E)$ denotes the density of states (DOS):

$$g(E) = \sum_{\text{Conf.}} \delta^{(1)}(H - E). \quad (2.7)$$

For KSAT theories $g(E)$ is integer valued, has finite support on the integer values of the compact interval $0 \leq E \leq M$ and an integral $\sum_E g(E) = 2^N$. A satisfiable Boolean form induces $g(E = 0) > 0$, while $g(E = 0) = 1$ corresponds to an \mathcal{F} that only has one unique satisfying assignment (USA). Boolean forms, that cannot be satisfied have $g(E = 0) = 0$. The quantity $g(E = 1)$ also is denoted the microcanonic phase space volume Ω_1 of the energy one energy surface.

Our knowledge of the statistical properties of K satisfiability stems from extensive analytical [3] and numerical studies [2] of random KSAT, which have demonstrated the existence of a transition, possibly a phase transition at values $\alpha_s(K)$. The SAT to UNSAT transition separates at low $\alpha < \alpha_s$ a phase where formulas \mathcal{F} are satisfied in the mean, from a phase at large $\alpha > \alpha_s$ where formulas \mathcal{F} can not be satisfied. Numerical data for the probability $0 \leq P_{\text{UNSAT}} \leq 1$ of un-satisfiable formulas within the mean of random KSAT are displayed in Fig.(2) and illustrate the statement. The data are of similar quality as the data obtained by Selman and Kickpatrick in 1996 [2]. The consensus is that probable realizations within random KSAT are 'hardest', i.e. computational most intractable, at and in the vicinity of the transition point $\alpha \approx \alpha_s$. However, this does not exclude the existence of still 'harder' i.e., worst case realizations which at arbitrary α are hidden in the tails of probability distribution functions for complexity related observables with small, possibly very small probabilities.

2.2. Search for Hard Problems

The starting point of our search for 'hard' realizations are observations that concern realizations with USA. If one considers USA realizations in 3SAT for the smallest spin number $N = 3$ and clause number M one inevitably arrives at the $M = 7 = 3 + 4$ realization

$$\begin{aligned} \mathcal{F}_{\text{USA}}(N = 3) = & \left(\begin{array}{ccccc} 1 & \vee & 2 & \vee & 3 \end{array} \right) \wedge \\ & \left(\begin{array}{ccccc} 1 & \vee & 2 & \vee & \bar{3} \end{array} \right) \wedge \\ & \left(\begin{array}{ccccc} 1 & \vee & \bar{2} & \vee & 3 \end{array} \right) \wedge \\ & \left(\begin{array}{ccccc} 1 & \vee & \bar{2} & \vee & \bar{3} \end{array} \right) \wedge \\ & \left(\begin{array}{ccccc} \bar{1} & \vee & 2 & \vee & 3 \end{array} \right) \wedge \\ & \left(\begin{array}{ccccc} \bar{1} & \vee & 2 & \vee & \bar{3} \end{array} \right) \wedge \\ & \left(\begin{array}{ccccc} \bar{1} & \vee & \bar{2} & \vee & 3 \end{array} \right) , \end{aligned} \quad (2.8)$$

which encodes the unique ground state $s_1 = s_2 = s_3 = +1$. This particular example is one of eight that all encode USA's for $N = 3$, and is turned in a readable form upon permuting clause and literal indices. It has interesting specific properties:

- FOR $N = 3$ \mathcal{F}_{USA} is the minimal form with a USA. For $N = 3$ and $M = 6$ there are no USA realizations in 3SAT.
- The density of states $g(E)$ only has two values $g(E = 0) = 1$ and $g(E = 1) = 7$. All spin flips acting on the ground-state lift the $E = 0$ energy surface by just one unit to $E = 1$. The states with $E = 1$ have dis-proportional large multiplicity and therefore $E = 0$ is hidden. This suggests that still 'minimal' but larger forms \mathcal{F}_{USA} at values $N > 3$ could inherit a similar property. These must exist at $\alpha = (N + 4)/N$ as one can introduce additional spins and clauses one by one. For example, if we introduce a fourth spin and extend \mathcal{F}_{USA} by one clause to an $(N, M) = (4, 8)$ form with comparable property, then

$$\mathcal{F}_{\text{USA}}(N = 4) = \mathcal{F}_{\text{USA}}(N = 3) \wedge \left(\begin{array}{ccccc} 4 & \vee & \bar{1} & \vee & \bar{2} \end{array} \right). \quad (2.9)$$

The latter form encodes the unique ground state $s_1 = s_2 = s_3 = s_4 = +1$ and has the density of states $g(E = 0) = 1$ and $g(E = 1) = 15$ respectively. Again $E = 1$ configurations have large multiplicity.

- Within \mathcal{F}_{USA} of eq.(2.8) there are exactly $m_1 = 3$ clauses - those with two negations - which in the unique solution are solved by just one true literal. There are in addition $m_2 = 3$ clauses which are solved by two literals and $m_3 = 1$ clauses which are solved by three literals. Also, there exists a polynomial transformation of 3SAT to maximal independent set (MIS) [13]. It is easy to show, that a unique ground-state of the 3SAT problem transforms into a degenerate ground-state in the corresponding MIS problem. The ground-state multiplicity MIS, $\Omega_{0,\text{MIS}}$, has the value

$$\Omega_{0,\text{MIS}} = 2^{m_2} 3^{m_3} = 24 \quad (3\text{SAT}, N = 3, M = 7), \quad (2.10)$$

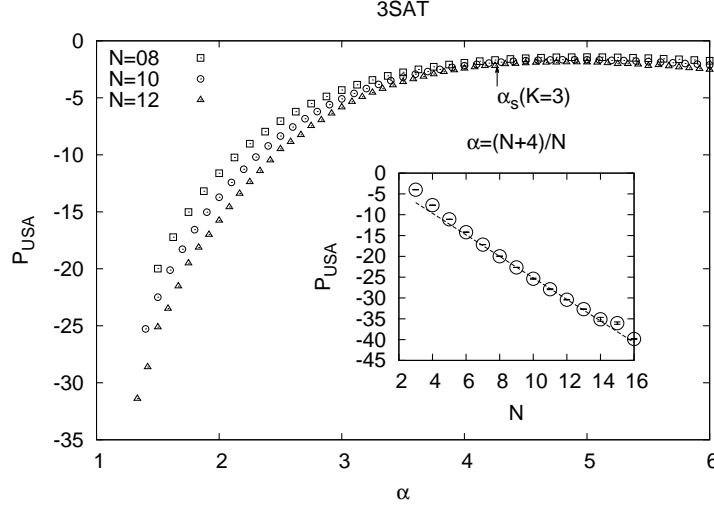


Figure 5: Probability P_{USA} of eq.(2.19) for the occurrence of problem realizations with unique satisfying assignment (USA) in 3SAT as a function of $\alpha = M/N$. Spin numbers are $N = 8, 10$ and $N = 12$. The inset of the figure displays the decrease of P_{USA} for α_{HARD} , see eq.(2.12) as a function of N .

on \mathcal{F}_{USA} . We note that m_1 of $\mathcal{F}_{USA}(N = 4)$ turns out to be $m_1 = 4$ while m_2 and m_3 remain having values $m_2 = 3$ and $m_3 = 1$, and thus also $\mathcal{F}_{USA}(N = 4)$ is constant at $\Omega_{0,MIS} = 24$. It is suggested that 'minimal' but larger ($N > 3$) forms \mathcal{F}_{USA} can have indices m_1 that are of magnitude $\mathcal{O}(N)$, which in turn limits the volume $\Omega_{0,MIS}$ to finite values. Finite values imply vanishing ground state entropy density $\ln \Omega_{0,MIS}/N$ under the polynomial transformation from 3SAT to MIS.

The existence of examples with interesting properties guides our expectations. The question is raised whether USA and 3SAT realizations at the ratio of clause to spin numbers

$$\alpha_{HARD} = \frac{N + 4}{N} \quad (2.11)$$

exist for arbitrary $N \geq 3$ and what their properties are? In absence of useful mathematical methods we use Monte Carlo simulations in order to actually construct members of the ensemble at α_{HARD} , and in a later measurement step we determine their properties. In particular we calculate Ω_1 , the multiplicity of the energy one surface. It is then necessary to employ biased Monte Carlo sampling techniques, as in the vicinity of $\alpha = 1$ USA realizations within random 3SAT have exponentially small probability. Finally it is easy to generalize our arguments to arbitrary K . For KSAT with $K \geq 2$ we expect USA realizations with minimum clause number at

$$\alpha_{HARD}(K) = \frac{N + 2^K - K - 1}{N}, \quad (2.12)$$

under the condition that $N \geq K$.

2.3. Monte Carlo Search and Checks

The Monte Carlo simulation performs a stochastic estimate of the biased partition function

$$\Gamma(\mu, W_{\text{MUCA}}) = \mathcal{N}^{-1} \sum_{\text{RANDOM KSAT}} e^{+W_{\text{MUCA}}(\mu)} \delta^{(1)}[\mu - g(E=0)], \quad (2.13)$$

which for $0 \leq \mu \leq 2^N$ is evaluated on the phase space of all possible random KSAT realizations for a given KSAT Hamiltonian eq.(2.5). The bias, as expressed by the Boltzmann factor $\exp[+W_{\text{MUCA}}(\mu)]$, is introduced along the lines of Multicanonical Ensemble simulations [11] and serves the purpose to lift the probabilities of rare μ configurations in the Markov chain. The Monte Carlo is expected to perform a random walk in μ and whenever the $\mu = 1$ sector is visited an ensemble member of $\langle \dots \rangle_{\text{HARD}}$ is stored on the disk of a computer. Our Monte Carlo is quite un-conventional and essential remarks are in order:

- The Markov chain of configurations consists of realizations as specified by their maps $i[\alpha, j]$ and frustration matrix $\epsilon_{\alpha, j}$. Each problem realization is attached to a Hamiltonian theory with density of states $g(E)$ that can be evaluated at $E = 0$, $\mu = g(E = 0)$. The calculation of μ for a given configuration unfortunately takes $\mathcal{O}(2^N)$ computational steps. Our Monte Carlo simulation therefore is limited to small numbers of spins. We studied KSAT theories for $K = 2, 3, 4, 5$ and $K = 6$. We were able to generate ensembles of 1000 statistical independent members each for maximum spin numbers $N_{\text{max}} = 18, 16, 14, 12$ and $N_{\text{max}} = 10$ respectively. Minimum spin numbers always are $N_{\text{min}} = K$.
- Configurations are updated with Metropolis updates [14]. The initial problem realization at μ_{I} is subject to a trial-update which targets μ_{F} . The Markov chain accept probability for the move is

$$P_{\text{ACC}} = \min[1, e^{+W_{\text{MUCA}}(\mu_{\text{F}}) - W_{\text{MUCA}}(\mu_{\text{I}})}], \quad (2.14)$$

and as usual, if the update is rejected the initial configuration stays within the Markov Chain.

- Trial updates are generated randomly on the space of random KSAT realizations. One chooses a random clause α_0 and clause position j_0 and at (α_0, j_0) trial values i_{Trial} and ϵ_{Trial} , which are uniformly distributed on the measure of the theory. The absence of redundancies and tautologies constrains the admissible move set. The typical number of Monte Carlo moves for the simulation of $\Gamma(\mu)$ is 10^9 . For the larger N values it was necessary to repeat the simulations with different random number sequences possibly 10, up to several 10 times. The numerical data, as presented in the paper, consumed one month of computer time on a 256 processor workstation cluster.

- The bias $W_{\text{MUCA}}(\mu)$ has to be chosen properly in order to guarantee efficient random walk behavior in the variable μ . In a preparation step we use Wang Landau simulations [10] to generate sufficiently accurate $W_{\text{MUCA}}(\mu)$ weight functions, which then enter the Multicanonical simulation of eq(2.13).

The biased partition function of eq.(2.13) serves as a tool to facilitate Monte Carlo sampling of different μ sectors in random KSAT and in particular the sector $\mu = 1$ (USA) is sampled efficiently. There is however an additional benefit. After finishing the biased Monte Carlo simulation a final reweighing step $\Gamma(W = 0) = \exp[-W(\mu)]\Gamma(W(\mu))$ restores the unbiased partition function

$$\Gamma(\mu) = \mathcal{N}^{-1} \sum_{\text{RANDOM KSAT}} \delta^{(1)}[\mu - g(E = 0)], \quad (2.15)$$

which on the space of random KSAT realizations simply counts the probability of $E = 0$ multiplicities μ . Given $\Gamma(\mu)$ we can determine expectation values of known observables within random KSAT, which provide consistency checks on the correctness of the Monte Carlo simulation. A list and a comparison to numerical data follows:

- In random KSAT there is always a finite probability of problem realizations with $E = 0$ non-vanishing multiplicity. In fact one can calculate the $E = 0$ mean multiplicity

$$\langle g(E = 0) \rangle_{\text{RANDOM KSAT}} = \langle \mu \rangle = \mathcal{N}^{-1} \sum_{\mu} \Gamma(\mu) \mu \quad (2.16)$$

on combinatorial grounds at arbitrary K exactly [12], which simply yields

$$\langle \mu \rangle = (1 - \frac{1}{2^K})^M 2^N. \quad (2.17)$$

In Fig.(3) we compare selected measurement data for $\langle \mu \rangle$ with the exact result for various values of K , N and M . The Monte Carlo data agree with the combinatorial result very well.

- One may wonder whether a theory with an entirely regular $\langle \mu \rangle$ will contain a non-regular structure at the SAT to UNSAT transition α_s . However, the constraint expectation value of the quantity $\frac{1}{N} \langle \ln \mu \rangle_{|\mu > 0}$, under omission of the $\mu = 0$ sector does in fact show non-trivial behavior. Within the SAT phase ($\alpha < \alpha_s$) it equals the ground-state entropy density $s_0 = \frac{1}{N} \langle \ln \mu \rangle$, for which long time ago [15] and for the theories 2SAT and 3SAT an α series-expansion was calculated within replica symmetry breaking theory up to order $\mathcal{O}(\alpha^{10})$. In Fig.(4) we compare our numerical data $\langle s_0 \rangle$ in 2SAT and 3SAT with the series expansions results. The figure contains two curves, which for 2SAT for $\alpha < \alpha_s = 1$ and for 3SAT for $\alpha < \alpha_s = 4.267$ are

indistinguishable from the numerical data points. Finally we note for random KSAT, that the probability P_{UNSAT} of an un-satisfiable formula has the simple representation

$$P_{\text{UNSAT}} = \mathcal{N}^{-1} \Gamma(\mu = 0). \quad (2.18)$$

The data are displayed in Fig.(2).

The main reason for the use of quite elaborate Monte Carlo techniques is the rareness of USA realizations for $\alpha \approx 1$, in particular for the conjectured exact point $\alpha = \alpha_{\text{HARD}}(K)$, as given in eq.(2.12). For all our theories with $K = 2, 3, 4, 5$ and $K = 6$ and for typical N like $N = 10$ we search the α -parameter space also at α -values below $\alpha_{\text{HARD}}(K)$ for USA realizations. Neither Multicanonical Ensemble simulations for several weight functions W_{MUCA} , nor Wang Landau simulations or, alternatively simulated annealing runs in μ - ever produced a USA realization for α below α_{HARD} . However, at α_{HARD} eq.(2.12) USA realizations are found. The relative probability P_{USA} for the occurrence of unique satisfying assignment's within random KSAT is

$$P_{\text{USA}} = \mathcal{N}^{-1} \Gamma(\mu = 1). \quad (2.19)$$

We display in Fig.(5) P_{USA} data in 3SAT for $N = 8, 10, 12$ spins. P_{USA} appears to be a slowly varying function above $\alpha_s = 4.267$, with a maximum around α_s and with a rapid decrease towards minimal and very small values at α_{HARD} and, problems with larger N appear to be increasingly improbable. The asymptotic decay of $P_{\text{USA}}(\alpha_{\text{HARD}})$ is consistent with an exponential decay $P_{\text{USA}}(\alpha_{\text{HARD}}) \propto \exp(-rN)$ with $r \approx 2.58$ in 3SAT and is depicted in the inset of Fig.(5). In addition at fixed spin number N values of $P_{\text{USA}}(\alpha_{\text{HARD}})$ turn out to be even smaller if larger K values are considered. We quote $\ln P_{\text{USA}}(\alpha_{\text{HARD}}) = -11.4, -31.39$ and $\ln P_{\text{USA}}(\alpha_{\text{HARD}}) \approx -84.3$ for the twelve spin theory with $K = 2, 3$ and in 4SAT. Finally we present for purposes of illustration a specific 3SAT realization for $N = 16$ spins and $M = 20$ clauses:

$$\begin{aligned} \mathcal{F}_{\text{USA}} = & (\overline{11} \vee 12 \vee \overline{3}) \wedge (\overline{14} \vee \overline{13} \vee \overline{8}) \wedge \\ & (11 \vee 2 \vee 12) \wedge (\overline{4} \vee 6 \vee 12) \wedge \\ & (6 \vee 12 \vee 13) \wedge (6 \vee 14 \vee \overline{7}) \wedge \\ & (\overline{8} \vee 6 \vee 9) \wedge (\overline{5} \vee \overline{12} \vee 3) \wedge \\ & (\overline{13} \vee \overline{16} \vee 4) \wedge (8 \vee 6 \vee 12) \wedge \\ & (3 \vee 12 \vee \overline{6}) \wedge (5 \vee 3 \vee \overline{12}) \wedge \\ & (15 \vee 5 \vee 12) \wedge (12 \vee 11 \vee \overline{3}) \wedge \\ & (6 \vee \overline{11} \vee 15) \wedge (\overline{15} \vee \overline{3} \vee \overline{12}) \wedge \\ & (\overline{13} \vee \overline{15} \vee 12) \wedge (15 \vee 16 \vee 10) \wedge \\ & (15 \vee \overline{3} \vee \overline{12}) \wedge (1 \vee 12 \vee \overline{9}) \end{aligned} \quad (2.20)$$

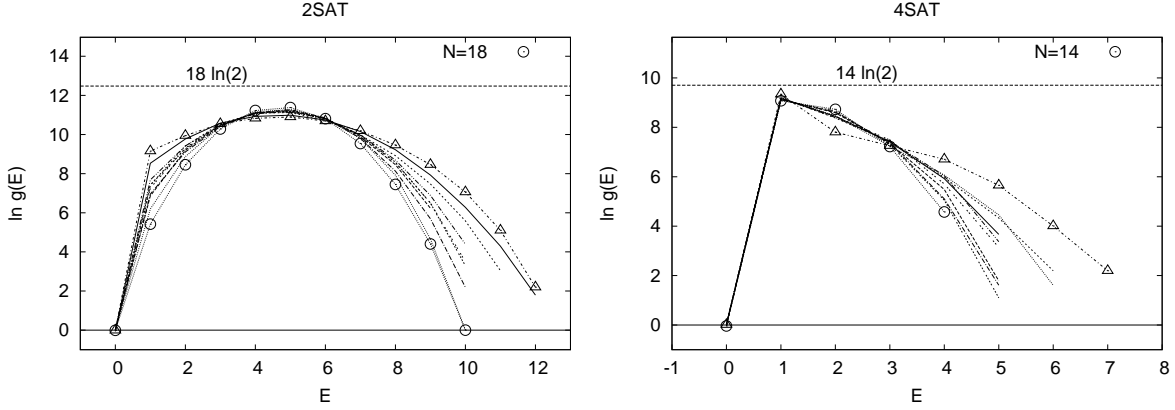


Figure 6: Ten density of states (DOS) curves in 2SAT (left) and 4SAT (right) for a number of spins $N = 18$ and $N = 14$ respectively.

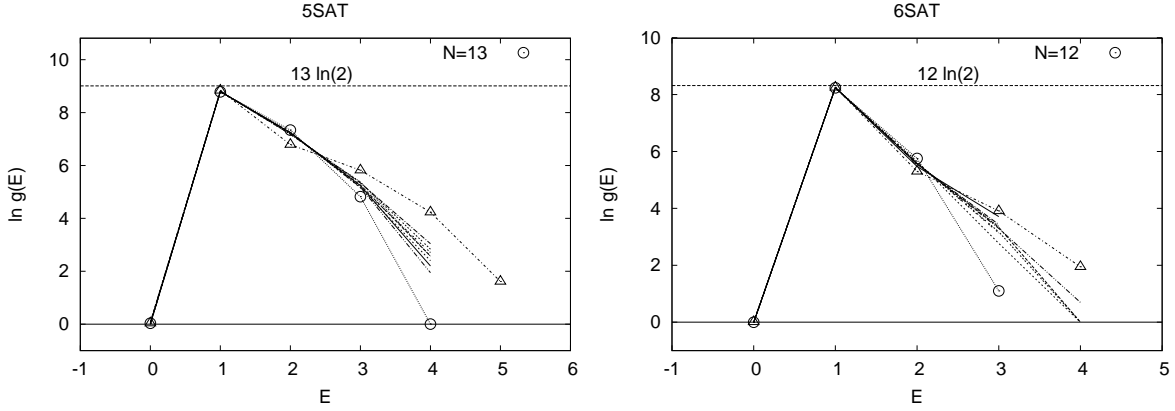


Figure 7: Ten density of states (DOS) curves in 5SAT (left) and 6SAT (right) for $N = 13$ and $N = 12$ respectively.

For $\alpha_{\text{HARD}} = 24/16 = 1.5$ it encodes the unique ground state 1100100111001000 - zero corresponding to spin down and one corresponding to spin up - and is characterized by the phase space volumes $\Omega_0 = 1$, $\Omega_1 = 19687$ and $\Omega_{0,\text{MIS}} = 24$. USA realizations for the given parameter values have probability $P_{\text{USA}} \approx 0.000000000000000004$ to occur by chance within random 3SAT. The full density of states of eq.(2.20) is depicted in Fig.(1), see the triangles in the figure. Finally the stochastic nature of the Monte Carlo search result is apparent if one compares the random structure of eq.(2.20) with the regular structure in eq.(2.8).

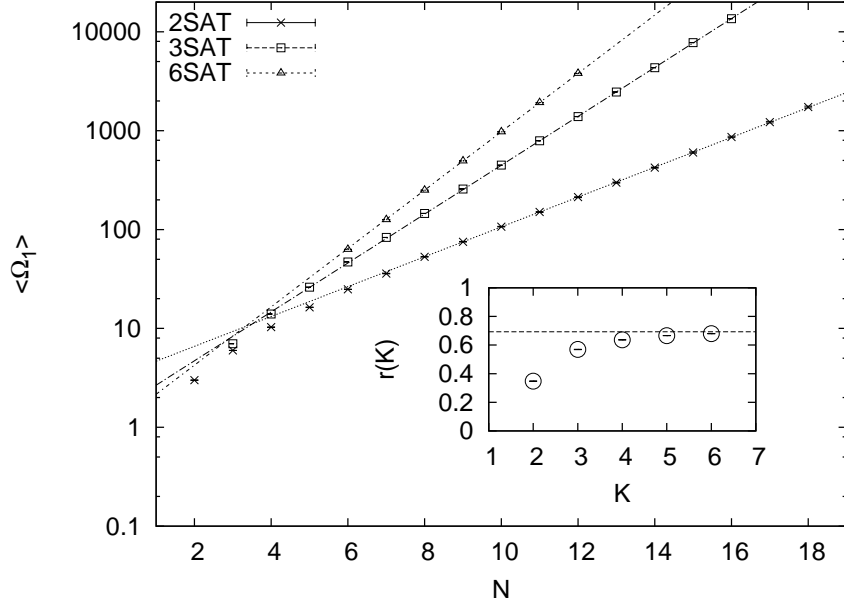


Figure 8: The mean density of states $\langle \Omega_1 \rangle$ on the energy one surface averaged in the hard problem ensemble $\langle \dots \rangle_{\text{HARD}}$ for the theories 2SAT, 3SAT and 6SAT in logarithmic scale as a function N .

K	$r(K)$	χ^2_{dof}
2	0.34762(112)	0.65
3	0.56918(096)	1.87
4	0.63620(015)	0.66
5	0.66574(025)	2.55
6	0.67934(014)	0.30

Table 1: Fit parameters of χ^2_{dof} fits to $\langle \Omega_1 \rangle$ data with the form eq.(3.2). The rate constants $r(K)$ approach the unstructured search value $\ln 2 = 0.6931\dots$ rapidly for large values of K .

3. Properties of Hard KSAT Realizations

For each of the generated problem realizations within the ensemble $\langle \dots \rangle_{\text{HARD}}$ and as defined by the partition function $\Gamma(\mu)$ of eq.(2.15) for $\mu = 1$, we calculate the density of states eq.(2.7). We determine its mean on the $E = 1$ surface

$$\langle \Omega_1 \rangle = \langle g(E = 1) \rangle_{\text{HARD}} . \quad (3.1)$$

Selected data for the density of states $g^\eta(E)$ with $\eta = 1, \dots, 10$ are displayed in Figures Fig.(6) and Fig.(7) for the $K = 2, 4, 5, 6$ KSAT theories. They complement the 3SAT data displayed in Fig.(1). In each case the multiplicity of $E = 1$ configurations exhibits a step $\Delta \ln \Omega = \ln \Omega_1 = \ln g(E = 1)$ that is of magnitude $\mathcal{O}(N)$ for the given number of spins N .

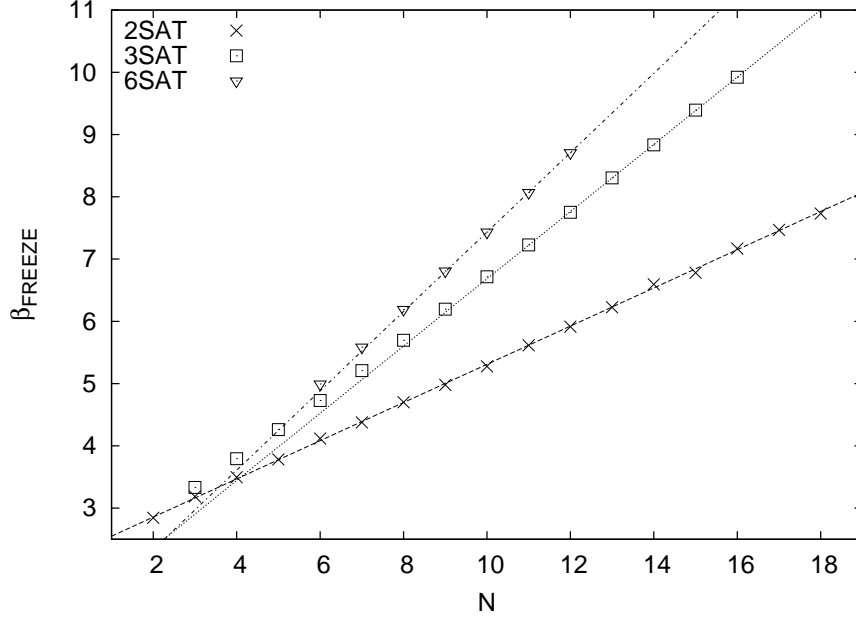


Figure 9: Position of the freezing transition in β_F , the inverse temperature. For large N values β_F asymptotically approaches values $\beta_F = \ln \Omega_1$ and thus the slopes the linear behavior approach values $r(K)$ as given in Table 1.

Our final numerical data for the mean multiplicity of $E = 1$ configurations $\langle \Omega_1 \rangle$, in the theories 2SAT, 3SAT and 6SAT are displayed in Fig.(8). The numerical data are consistent with an exponential growth

$$\langle \Omega_1 \rangle = \text{const } e^{+r(K)N}, \quad (3.2)$$

for large values of N with finite growth rate constants $r(K)$. Subsequently, we performed χ^2_{dof} fits to the $\langle \Omega_1 \rangle$ data in order to determine the shape of the singularity eq.(3.2) and to measure values of the rate constants $r(K)$ in KSAT theories with $K = 2, 3, \dots, 6$. Restricting the fit interval to the cases with $N \geq 10$ we obtain acceptable χ^2_{dof} -values for the fit. The final rate constants $r(K)$ and χ^2_{dof} -values of the fits are contained in Table 1. The K -dependence of the rate constants $r(K)$ is also depicted in the inset of Fig.(8). Starting from a moderate value for the rate constant in 2SAT, $r(K = 2) = 0.348(2)$, we obtain $r(K = 3) = 0.54(1)$ in 3SAT and, beyond $K = 3$ the rate constants rapidly approach the unstructured search value $r = \ln 2 = 0.6931\dots$. For 6SAT the rate constant is $r(K = 6) = 0.6793(2)$.

A classical statistical model with a density of states $g(E)$, that squeezes an exponential large number of configurations into the first energy level above the ground-state, see the right panel of Fig.(7) is certainly a very special theory. Let us recall the ferromagnetic Ising model, which in any dimension D has a ground-state degeneracy $g(E = 0) = 2$ as well as a multiplicity $\Omega_1 = g(E = 2D) = 2N$ at the first energy level. Polynomial singularities in Ω_1 are the consequence of theories with local interactions. However, the class of problems

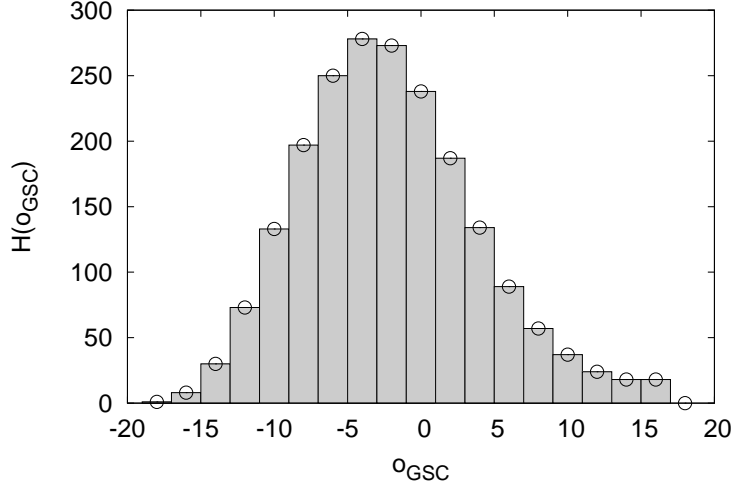


Figure 10: Overlap distribution to the ground state in accord with eq.(3.3) for a single $N = 18$ problem in 2SAT.

considered here does not possess this property.

The spin configurations at energy $E = 1$ will have a phase space distribution and it is interesting to know, whether that distribution is biased towards the ground state configuration. For this purpose we calculate the overlap to the ground state

$$o_{\text{GSC}} = \sum_{i=1}^N s_i s_i^0 \quad (3.3)$$

where s_i^0 denotes ground state spins. For purposes of illustration we display in Fig.(10) the number histogram $H(o_{\text{GSC}})$ for a single $N = 18$ problem in 2SAT. We obtain a bell-shaped overlap distribution which actually is slightly biased away from the ground state to the negative half space. We note that the histogram carries entries at $o_{\text{GSC}} = 16$ and thus the ground state is accessible via single spin flips from the $E = 1$ surface. We also have analyzed the connectivity of $E = 1$ configurations. Using *ballistic shooting* we find that any two $E = 1$ configurations are connected by sequences of single spin flips without leaving $E = 1$. This is different from spin glasses where in general there are several connectivity components and corresponding free energy barriers. Any single spin flip dynamics e.g. Metropolis updates can easily explore the $E = 1$ surface.

We also consider the canonical ensemble eq.(2.6). We calculate the internal energy $\langle E \rangle = \langle U \rangle_{\text{HARD}}$ with $U = \partial_{\beta} \ln Z$, as well as the specific heat $\langle C_V \rangle(\beta) = \langle \beta^2 \partial_{\beta}^2 U \rangle_{\text{HARD}}$, as a function of the inverse temperature $\beta = T^{-1}$. For 3SAT we display $\langle E \rangle$ and $\langle C_V \rangle$ for $N = 4, 8$ and $N = 16$ spins in Fig.(11). A theory with a finite energy gap is expected to possess a freezing phase transition at low, possibly very low temperatures T_F below which and for values $T < T_F$ the internal energy approaches its

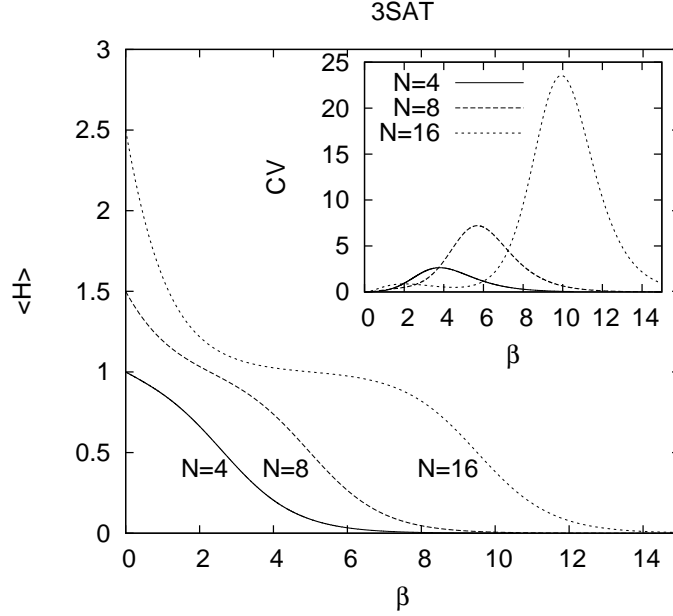


Figure 11: Expectation value $\langle E \rangle$ of the energy in 3SAT as a function of the inverse temperature $\beta = 1/T$. The inset displays specific heat $\langle C_V \rangle$ data. At the freezing transition marked by the position of the maximum of the specific heat an exponentially large number Ω_1 of energy $E = 1$ configurations coexists with the single ground-state at $E = 0$.

asymptotic ground-state value $\langle E \rangle = 0$. The numerical data in fact confirm the presence of freezing, with a position as given by the position of a pronounced peak in the specific heat, see the inset of Fig.(11). Figure (9) displays $\beta_F = T_F^{-1}$ data in 3SAT, which as a function of N exhibit a blatant linear dependence, see the straight lines in Fig.(11). We remark that at the freezing point configurations with $E = 1$ coexist with a single configuration at the ground-state energy.

A popular algorithm within the canonical ensemble for the solution of optimization problems is simulated annealing (SA) [16]. Simulated annealing runs will have to use temperature annealing schedules with temperatures low enough to reach the freezing point at T_F e.g. $T \approx 0.1$ for 16 spins in 3SAT and, then will have to explore Ω_1 number of possibilities to finally arrive at the ground-state. The process will consume an exponentially large amount of time, if Ω_1 is exponentially large. We do not expect, that other algorithmic improvements like kinetic Monte Carlo methods [17] can avoid the exponential singularity.

We have implemented simulated annealing for the problem set in 3SAT. We use the canonical partition function eq.(2.6) and choose a random initialized spin-configuration. We then perform local Metropolis spin updates in a multi-spin coded computer program [18, 19]. We employ compute time farming on a parallel computer with a parallel random number generator of Marsaglia [20]. Each annealing trajectory is started at the very high temperature

$$T_0 = 100 \quad (3.4)$$

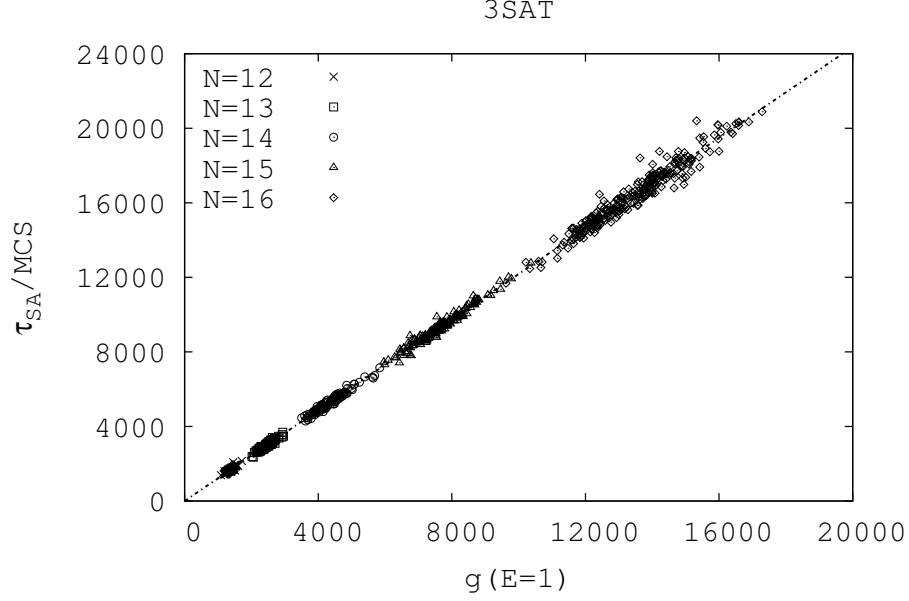


Figure 12: 3SAT correlation of run times in simulated annealing eq.(3.7) with the density of states $g(E = 1)$. We combine run-times at various N into a single plot. Plotted is a subset of the set of all problems.

and terminates after 1000 Sweeps i.e., $1000 \times N$ Monte Carlo steps where N is the spin number, at the exact temperature

$$T_{\text{End}} = \frac{1}{30}. \quad (3.5)$$

We use a polynomial temperature schedule

$$T_i = a i^{-b} \quad (3.6)$$

where i is the sweep number $i = 1, \dots, 1000$ and constants a, b are determined to meet the boundary conditions on the temperature. For each problem we repeat the annealing trajectories 6400 times with different random numbers and determine the mean success probability $P_{\text{Success}}^{\text{SA}}$ with $0 \leq P_{\text{Success}}^{\text{SA}} \leq 1$ of successful ground-state searches after the sweep 1000 has been finished. Our measure of SA search run-time is

$$\tau_{\text{SA}} = \frac{\ln[1 - P_{\text{Target}}^{\text{SA}}]}{\ln[1 - P_{\text{Success}}^{\text{SA}}]} \times 1000 \times N \text{ [Monte Carlo Steps]} \quad (3.7)$$

at target success rate one-half : $P_{\text{Target}} = \frac{1}{2}$. The procedure is repeated for a possible 1000 realizations and at all values of N . The correlation of run-times τ_{SA} with the density of states $g(E = 1)$ is linear for 3SAT, as can be inspected in Fig.(12) for a selected set of problems at various N . These run times are quite short. If e.g. at $N = 16$ the energy surface has 16000 degenerate spin configurations a typical number of $\mathcal{O}(20000)$ Monte Carlo Steps is

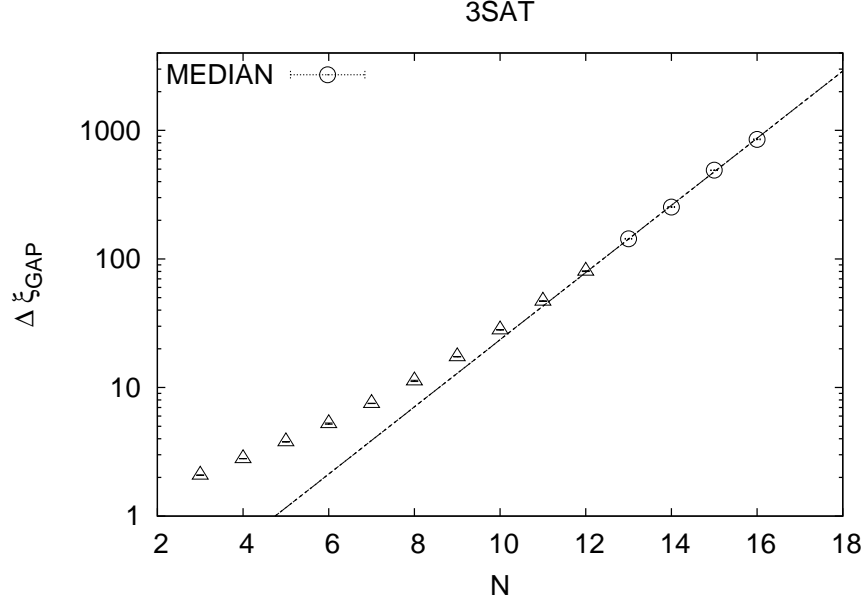


Figure 13: Preliminary quantum gap-correlation length values $\Delta \xi_{GAP}$ at the quantum phase transition of Z_Q in eq.(1.1).

sufficient to solve the problem at a success rate of one half. However if the target success rate is demanded to be very close to unity larger times are needed. Our findings imply that the classical compute time for solving problems with simulated annealing goes like $\tau_{\text{Classical}} \propto e^{+r(K)N}$ with values $r(K)$ as given in Table 1. It is this kind of singularity a quantum search has to compete with.

4. Conclusion

Within the scope of the present work, we have generated prototype problem realizations within KSAT theories, which under the constraint of a unique satisfying assignment (USA) at minimal clause number develop extremal statistical properties. The phase space volume Ω_1 at the minimal energy gap is exponentially large and likewise for a given KSAT theory maximal. The idea was formulated in 2005 by Znidaric [9] but in absence of efficient Monte Carlo methods it was not worked out at minimal clause number and at large values of the rate constants $r(K)$. The class of problems as presented here exemplifies our current understanding of physical search complexity in random systems in a straight and simple way: A single ground state is hidden in an exponentially large phase space volume at the first energy gap. For the theories with large K almost all spin configurations are collapsed to the $E = 1$ surface, except the one ground state configuration at $E = 0$. In this situation there exists no distance measure or cluster property which within the $E = 1$ surface would allow the detection of a direction, as to where the ground state could be searched for. Representatives

of the ensemble $\langle \dots \rangle_{\text{HARD}}$ can be obtained at request from the author.

The given problems at $K = 3, 4, 5$ and $K = 6$ in this work are constructed on problem Hamiltonians that contain higher order interactions of spins like $a_{i,j,k} s_i s_j s_k$. From a physics point of view it would possibly be nicer to eliminate such unphysical couplings and stay with only 2-point spin couplings, as well as magnetic fields. We mention that all the Hamiltonians at $K \geq 3$ can be transformed via polynomial transformations to Maximal Independent Set (MIS), see [13], which in fact can be represented by 2-point and magnetic field spin couplings only. It is plausible to assume that these after polynomial transformation retain their “hardness”.

The design of problem realizations with specific properties facilitates the subsequent study of proper defined search efficiency’s in processes, that can possibly be implemented on a physical device e.g., a quantum computer. For purposes of illustration we mention here quantum annealing within the quantum partition function Z_Q of eq.(1.1). Search times for ground-state calculations via quantum annealing are expected to be bounded by below through a gap-correlation length $\Delta\xi_{GAP}$, which is determined from spin-spin correlations along the imaginary Trotter Suzuki time of Z_Q at the quantum critical point. For 3SAT we present in Fig.(13) preliminary numerical results for $\Delta\xi_{GAP}$ in the median average of the hard problem ensemble. The data, as indicated by the straight line in the figure, show in fact also an exponential singularity $\Delta\xi_{GAP} \propto \exp[+r_Q N]$ of a similar type as in eq.(3.2), that now is governed by a quantum rate constant $r_Q \approx 0.60(1)$, a value that is close to $r(K=3) = 0.569(1)$ of Table 1. The caveat however is, that in presence of a Landau Zener avoided level crossings quantum run-times for linear quantum annealing schedules show a quadratic singular behavior $\tau_{\text{Quantum}} \propto \Delta\xi_{GAP}^2$ [21], which leaves the quantum search efficiency far behind the classical search. Similar exponential singularities at smaller values of r_Q were already observed for quantum 3SAT on a set of ‘weaker’ problems [7]. A detailed study of quantum search complexities on the set of hard problems in 2SAT has just been completed [22] and complements the less physical findings of this work.

Finally we mention that the spin numbers N in this work are embarrassing small, as the Monte Carlo search on the problem set consumes exponentially large resources. We can safely say that with current methods it is not possible to generate a corresponding ensemble of problems even for spin numbers as small as $N = 30$. It is however not excluded, that single problem representatives can be found by clever heuristic construction. We emphasize that we do not want to give up the ensemble property because otherwise we would be studying arbitrary mathematical problems. This will be relevant for search complexity distributions which are expected to exhibit ensemble properties.

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